Technische Universität Berlin

Total-Variation-Based Phase Retrieval in Optical Diffraction Tomography

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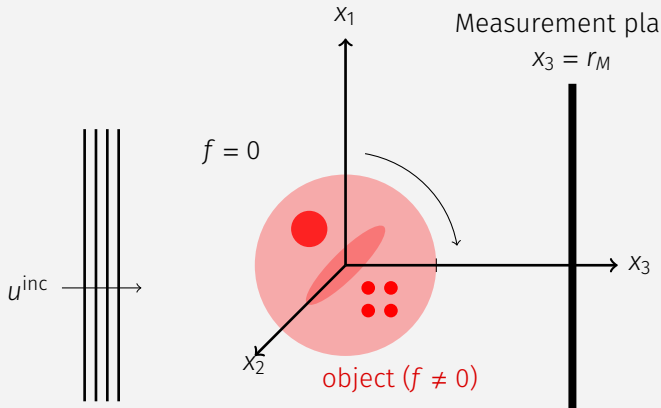
Optical Diffraction Tomography (ODT)

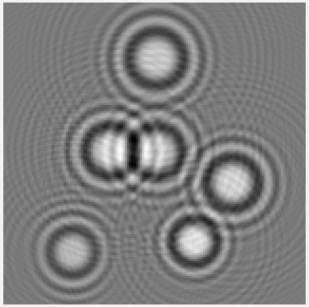


Incident field:
Plane wave with normal x_3

[Kirisits, Quellmalz, Ritsch-Marte, Scherzer, Setterqvist, Steidl, 2021]

Optical Diffraction

- Optical diffraction occurs when the wavelength is large compared with the object.



Simulation of the scattered field from spherical particles (size ≈ wavelength)

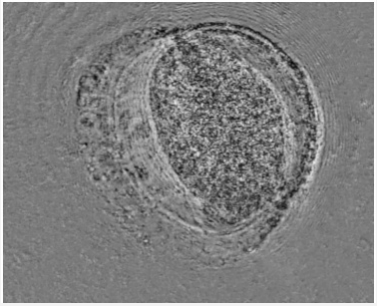


Image with diffraction
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Modelling Optical Diffraction

- Object illuminated by plane wave $u^{\text{inc}}(\boldsymbol{x}) = \mathrm{e}^{\mathrm{i}k_0 x_3}$.
- Total field $u^{\text{tot}}(\boldsymbol{x}) = u^{\text{sca}}(\boldsymbol{x}) + u^{\text{inc}}(\boldsymbol{x})$ solves the wave equation

$$-\left(\Delta + f(\boldsymbol{x}) + k_0^2\right) u^{\text{tot}}(\boldsymbol{x}) = 0.$$

- Rearranging yields

$$-\left(\Delta + k_0^2\right) u^{\text{sca}}(\boldsymbol{x}) - \underbrace{\left(\Delta + k_0^2\right) u^{\text{inc}}(\boldsymbol{x})}_{=0} = f(\boldsymbol{x}) \left(u^{\text{sca}}(\boldsymbol{x}) + u^{\text{inc}}(\boldsymbol{x})\right).$$

Born Approximation

Assuming $|u^{\text{sca}}| \ll \left|u^{\text{inc}}\right|$, we obtain

$$-\left(\Delta + k_0^2\right) u^{\text{sca}}(\boldsymbol{x}) = f(\boldsymbol{x}) u^{\text{inc}}(\boldsymbol{x})$$

- **Given Data:** $u^{\text{tot}}(x_1, x_2, r_{\text{M}})$ at measurement plane $x_3 = r_{\text{M}}$ for different times $t \geq 0$.
- **Aim**: Recover the scattering potential $f(\boldsymbol{x})$ with $\operatorname{supp} f \subset \mathcal{B}_{r_{\text{M}}} \subset \mathbb{R}^3$.

Fourier Diffraction Theorem

1. Scattering potential $f \in L^p$, $p > 1$, where $\mathbf{supp}(f) \subset \mathcal{B}_{r_M}$, $0 < r_M$.
2. Incident field is a plane wave $u^{\text{inc}}(\boldsymbol{x}) = \mathrm{e}^{\mathrm{i}k_0 x_3}$.
3. Born approximation is valid and u^{sca} satisfies the Sommerfeld condition (u^{sca} is an outgoing wave).
4. Scattered field u^{sca} is measured at the plane $x_3 = r_M$.

Then, the scattered field is approximated by

$$\sqrt{2/\pi}\,\kappa \mathrm{i}\,\mathrm{e}^{-\mathrm{i}\kappa r_M}\,\mathcal{F}[u_t^{\text{sca}}(\cdot,\cdot,r_M)](k_1,k_2) = \mathcal{F}[f](R_t \boldsymbol{h}(k_1,k_2)),$$

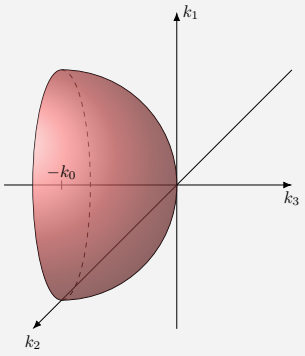
where

$$\boldsymbol{h}(k_1,k_2) := (k_1,k_2,\kappa(k_1,k_2)-k_0)^{\mathsf{T}}$$

and

$$\kappa(k_1,k_2) := \sqrt{k_0^2-k_1^2-k_2^2}$$

for $k_1^2+k_2^2 \le k_0^2$.



Hemisphere $\boldsymbol{h}(\boldsymbol{k})$

ODT Inversion

Theorem (ODT inversion)

Let $f \in L^1(\mathbb{R}^d)$ have a compact support in $\mathcal{B}^d_{r_M}$, and let the Lebesgue measure of

$$\mathcal{Y} \coloneqq \{R_t \boldsymbol{h}(\boldsymbol{y}') : \boldsymbol{y}' \in \mathcal{B}^{d-1}_{k_0},\ t \in [0, T]\} \subset \mathbb{R}^d$$

be positive. Then f is uniquely determined by the given data.

Proof.

- Exploit the Fourier diffraction theorem to obtain $\mathcal{F}[f]$ on $\mathcal{Y}$.
- Apply Paley–Wiener to extend $\mathcal{F}[f]$ to $\mathbb{R}^d$.
- Use the uniqueness of the Fourier transform.

Proposition (Paley–Wiener)

Let $f \in L^1(\mathbb{R}^d)$ have compact support. Then the Fourier transform $\mathcal{F}[f] \in C(\mathbb{R}^d)$ is uniquely extendable to an analytic function on $\mathbb{C}^d$.

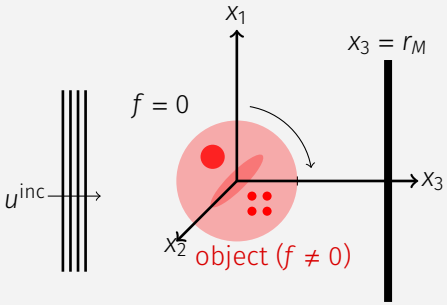
Discretization

- Index set $\mathcal{I}_K := \{-K/2, \dots, K/2 - 1\}$.
- Object discretization:

$$f_{\boldsymbol{k}} := f(\boldsymbol{x}_{\boldsymbol{k}}) \quad \text{with} \quad \boldsymbol{x}_{\boldsymbol{k}} := \tfrac{2L_S}{K}\boldsymbol{k}, \quad \boldsymbol{k} \in \mathcal{I}_K^3$$

- Measurement discretization:

$$u^{\mathrm{tot}}_{t_m}(\boldsymbol{y}_{\boldsymbol{n}}, r_M), \quad \text{with} \quad \boldsymbol{y}_{\boldsymbol{n}} := \tfrac{2L_M}{N}\boldsymbol{n}, \quad \boldsymbol{n} \in \mathcal{I}_N^2.$$



- Discrete Fourier Transform (DFT):

$$\left[F_{\mathrm{DFT}}\, u^{\mathrm{sca}}_{t_m}\right]_{\boldsymbol{\ell}} := \sum_{\boldsymbol{n} \in \mathcal{I}_N^2} u^{\mathrm{sca}}_{t_m}(\boldsymbol{y}_{\boldsymbol{n}}, r_M)\, \mathrm{e}^{-2\pi \mathrm{i} \boldsymbol{n} \cdot \boldsymbol{\ell}/N}, \qquad \boldsymbol{\ell} \in \mathcal{I}_N^2.$$

- Non-uniform Discrete Fourier Transform (NDFT):

$$[F_{\mathrm{NDFT}} \boldsymbol{f}]_{m,\boldsymbol{\ell}} := \sum_{\boldsymbol{k} \in \mathcal{I}_K^3} f_{\boldsymbol{k}}\, \mathrm{e}^{-\mathrm{i} \boldsymbol{x}_{\boldsymbol{k}} \cdot (R_{t_m} \boldsymbol{h}(\boldsymbol{y}_{\boldsymbol{\ell}}))}, \qquad \boldsymbol{\ell} \in \mathcal{I}_N^2.$$

Discretization

Fourier Diffraction Theorem:

$$\sqrt{2/\pi}\,\kappa \mathrm{i}\,\mathrm{e}^{-\mathrm{i}\kappa r_{\mathrm{M}}}\,\mathcal{F}[u_t^{\mathrm{sca}}(\cdot,\cdot,r_{\mathrm{M}})](k_1,k_2) = \mathcal{F}[f](R_t \boldsymbol{h}(k_1,k_2)).$$

Discretized Forward Operator

The forward operator may be discretized by

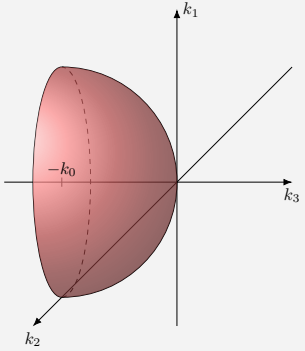
$$\boldsymbol{D}_{t_m}^{\mathrm{tot}}[\boldsymbol{f}] := \boldsymbol{F}_{\mathrm{DFT}}^{-1}(\boldsymbol{c} \odot [\boldsymbol{F}_{\mathrm{NDFT}}[\boldsymbol{f}]]_m) + \mathrm{e}^{\mathrm{i}k_0 r_{\mathrm{M}}}$$

with

$$\boldsymbol{c} = \left[\frac{\mathrm{i}}{\kappa(\boldsymbol{y}_{\boldsymbol{\ell}})}\,\mathrm{e}^{\mathrm{i}\,\kappa(\boldsymbol{y}_{\boldsymbol{\ell}})\,r_{\mathrm{M}}}\,(N/L_{\mathrm{M}})^{d-1}(L_{\mathrm{S}}/K)^d\right]_{\boldsymbol{\ell}\in\mathcal{G}_N^2}.$$

[Kirisits, Quellmalz, Ritsch-Marte, Scherzer, Setterqvist, Steidl, 2021]

- The NDFT computes the data on all hemispheres simultaneously.



Hemisphere $\boldsymbol{h}(\boldsymbol{k})$

Discretized Backward Operator

Input: Scattered wave $\boldsymbol{v}^{\mathrm{sca}}_{m,\boldsymbol{n}} \coloneqq u^{\mathrm{tot}}_{t_m}\left(\boldsymbol{n}\frac{2L_{\mathrm{M}}}{N}, r_{\mathrm{M}}\right) - \mathrm{e}^{k_0 r_{\mathrm{M}}}$, $\boldsymbol{n} \in \mathcal{G}_N^{d-1}$

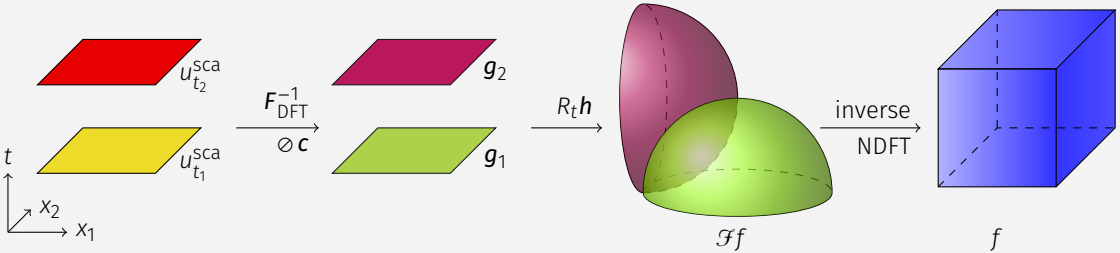
for $m = 1, \ldots, M$

$\tilde{\boldsymbol{g}}_m \coloneqq \boldsymbol{F}_{\mathrm{DFT}} \boldsymbol{v}^{\mathrm{sca}}_m$

$\boldsymbol{g}_m \coloneqq \tilde{\boldsymbol{g}}_m \oslash \boldsymbol{c}$, where $\oslash$ is the Hadamard (entrywise) division

Compute the inverse NDFT by solving $\boldsymbol{F}_{\mathrm{NDFT}} \boldsymbol{f} = \boldsymbol{g}$ for $\boldsymbol{f}$

Output: Scattering potential $\boldsymbol{f} \approx [f(\boldsymbol{x}_{\boldsymbol{k}})]_{\boldsymbol{k} \in I_K^d}$



Inversion of the NDFT

1. Backpropagation.
2. Conjugate Gradients (CG) on the normal equations:

$$\operatorname*{arg\,min}_{f \in \mathbb{R}^{K^d}} \quad \|F_{\mathrm{NDFT}}[f] - g\|_2^2.$$

3. Regularized inverse:

$$\operatorname*{arg\,min}_{f \in \mathbb{R}^{K^d}} \quad \chi_{\mathbb{R}^{K^d}_{\geq 0}}[f] + \tfrac{1}{2}\|F_{\mathrm{NDFT}}(f) - g\|_2^2 + \lambda \mathrm{TV}(f)$$

with total variation

$$\mathrm{TV}(f) := \sum_{k \in \mathcal{I}_K^3} \|\operatorname{grad} f(x_k)\|_2.$$

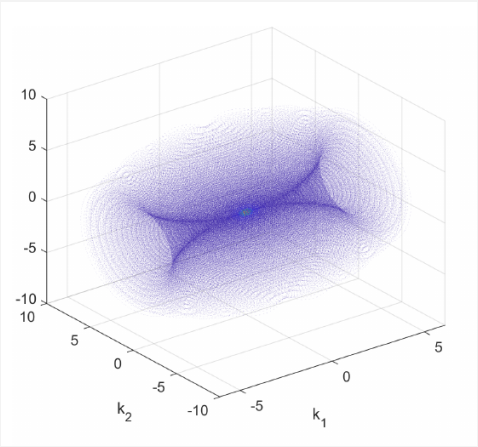
- Use the primal-dual (PD) iteration [Chambolle & Pock 2010].
- Adaptive selection of step sizes [Yokota & Hontani 2017].

Test Setup

- Use normalized wavelength 1, ie $k_0 = 2\pi$.
- 3D test function f is given analytically.
- Generate simulated data via convolution with the Green function (different discretization of the Born approximation).
- Fix the rotation axis initially.
- This leads to 'missing cones.'
- Employ the NFFT (Non-uniform fast Fourier transform) for computing $F_{\mathrm{NDFT}}[f]$ in $\mathcal{O}(N^3 \log N)$ steps.

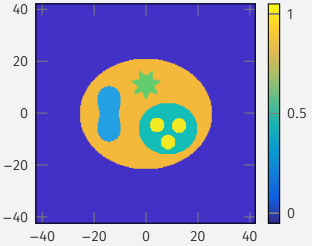
[Dutt, Rokhlin, 1993], [Beylkin, 1995],

[Potts, Steidl, Tasche, 2001], [Potts, Kunis, Keiner, 2004+]

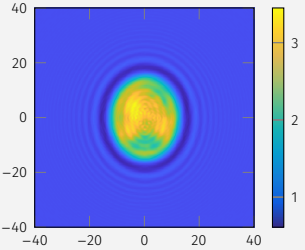


Simulated data: Fourier transform $|\mathcal{F}f|$ at 496944 nodes (constant rotation axis)

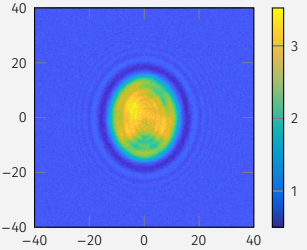
Test Data



Ground truth f
($240 \times 240 \times 240$ grid)
Slice at $x_3 = 0.35$

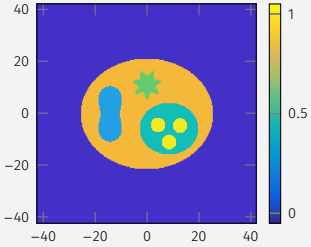


Exact data $\left|u_t^{\text{tot}}(\cdot, r_M)\right|$
240×240 grid
240 rotations

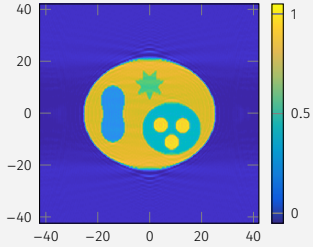


5 % Gaussian noise

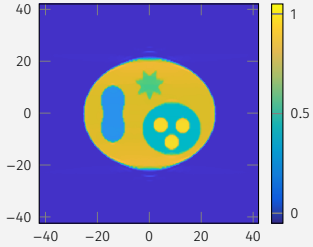
Exact Data Inversion



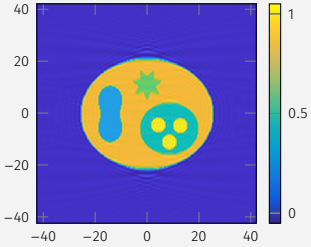
Ground truth



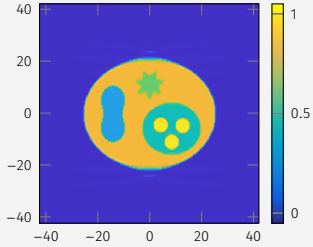
Backpropagation (BP)
PSNR 29.07, SSIM 0.614, 4 sec



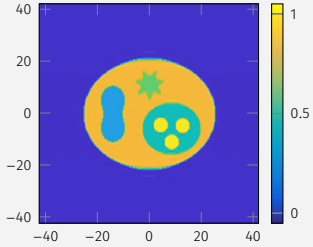
BP + TV denoising
PSNR 32.79, SSIM 0.987, 37 sec



Conjugate Gradient (CG)
PSNR 33.36, SSIM 0.955, 79 sec

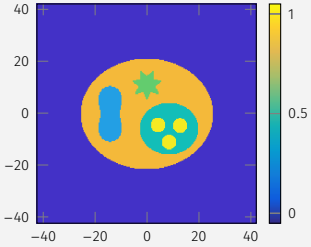


CG + TV denoising
PSNR 33.82, SSIM 0.988, 31 sec

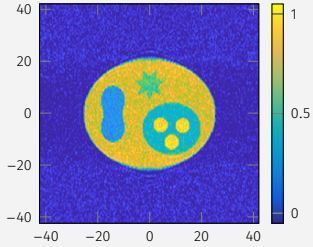


Primal-Dual (PD) with TV
PSNR 34.36, SSIM 0.957, 21 min

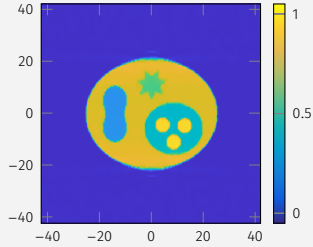
Noisy Data Inversion



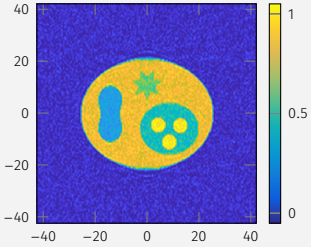
Ground truth



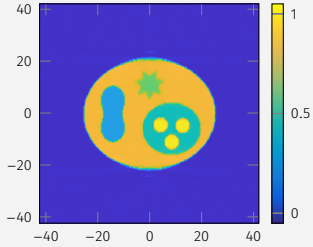
Backpropagation (BP)
PSNR 24.53, SSIM 0.178



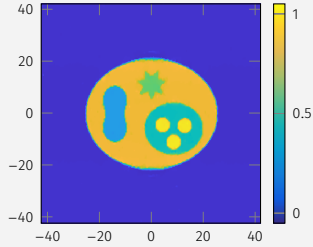
BP + TV denoising
PSNR 32.51, SSIM 0.968



Conjugate Gradient (CG)
PSNR 26.74, SSIM 0.309



CG + TV denoising
PSNR 33.53, SSIM 0.965



Primal-Dual (PD) with TV
PSNR 33.58, SSIM 0.736

Phase Retrieval in ODT

- In practice, one can often only measure the intensity

$$|u_t^{\mathrm{tot}}(y, r_{\mathrm{M}})| = |u_t^{\mathrm{sca}}(y, r_{\mathrm{M}}) + e^{ik_0 r_{\mathrm{M}}}|.$$

- Existing phase retrieval methods in diffraction tomography
  - require more measurements [Gbur, Wolf, 2002], [Wedberg, Stamnes, 1995],
  - use far zone approximations [Cheng, Han, 2001] [Gureyev, Davis, 2004],
  - consider phase retrieval separate from reconstruction [Maleki, Devaney, 1993],
  - use techniques of ptychography [Horstmeyer, Chung, Ou, Zheng, Yang 2016].

- We have additional information:
  - f is real and non-negative,
  - f has bounded support,
  - f is piecewise constant.
- Uniqueness guarantees are not available yet.

Hybrid Input-Output (HIO) Algorithm

Input: $\boldsymbol{d} = |\boldsymbol{D}[\boldsymbol{f}]|$, $\beta \in [0,1]$, $r_s > 0$

Initialize $\boldsymbol{g}^{(0)} := \boldsymbol{d}$

for $j = 0, 1, 2, \ldots$

$$\boldsymbol{f}^{(j)} := \boldsymbol{D}^{-1}[\boldsymbol{g}^{(j)}]$$

$$\tilde{f}_k^{(j)} := \begin{cases} \max\{f_k^{(j)}, 0\}, & \|\boldsymbol{x}_k\|_2 \le r_s \\ 0, & \|\boldsymbol{x}_k\|_2 > r_s \end{cases}$$

$$f_k^{(j+1/2)} := \begin{cases} f_k^{(j)}, & \text{if } f_k^{(j)} = \tilde{f}_k^{(j)} \\ f_k^{(j-1/2)} - \beta(f_k^{(j)} - \tilde{f}_k^{(j)}), & \text{otherwise} \end{cases}$$

$$\boldsymbol{g}^{(j+1/2)} := \boldsymbol{D}[\boldsymbol{f}^{(j+1/2)}]$$

$$\boldsymbol{g}^{(j+1)} := \boldsymbol{d}\,\mathrm{sgn}(\boldsymbol{g}^{(j+1/2)})$$

Output: Approximate scattering potential $\boldsymbol{f}^{(j)}$

Reducing Computational Complexity

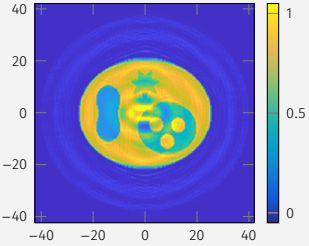
- Outer loop with HIO and inner loop with primal-dual (PD).
- Both algorithms often show slow convergence.

Improvements

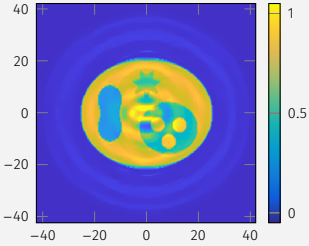
- Restart primal-dual with the parameters dual variable from the previous outer step.
- Use faster HIO/CG to obtain a starting solution for primal-dual.
- Use fast FFT and NFFT algorithms.
- Employ weights from the backpropagation to the minimization problem.

Code available on Github: `https://github.com/michaelquellmalz/FourierODT`

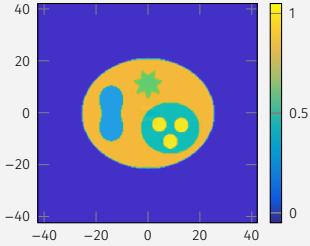
Exact Phase Retrieval



HIO/CG reconstruction
$J_{IO} = 10$, $J_{CG} = 5$
PSNR 29.52, SSIM 0.713
5 min

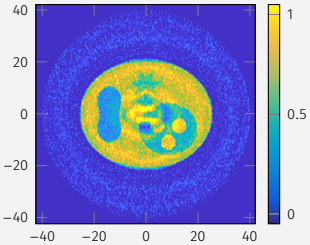


HIO/CG + TV denoising
$\lambda = 0.02$, $J_{TV} = 20$
PSNR 29.88, SSIM 0.713
31 sec

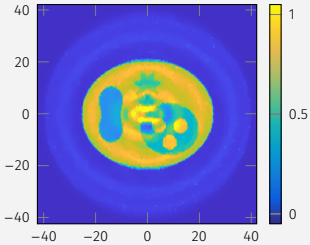


HIO/PD with TV
λ=0.01, J_{IO}=200, J_{PD}=5
PSNR 34.92, SSIM 0.994
3 h 48 min

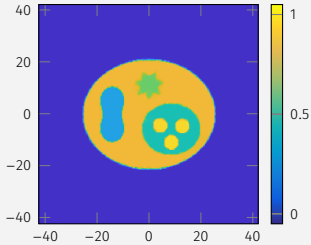
Noisy Phase Retrieval (5 % Gaussian)



HIO/CG reconstruction
$J_{IO} = 10$, $J_{CG} = 5$
PSNR 24.71, SSIM 0.589



HIO/CG + TV denoising
$\lambda = 0.05$, $J_{PD} = 20$
PSNR 27.16, SSIM 0.623



HIO/PD with TV
λ=0.05, J_{IO}=200, J_{PD}=5
PSNR 34.10, SSIM 0.993

Summary/Outlook

- Using the Born approximation and the Fourier diffraction theorem to model ODT.
- Total-variation-based regularized inversion of the NDFT.
- Hybrid input-output algorithms for phase retrieval.

- How to ensure uniqueness in ODT phase retrieval.
- How to recover the rotations in advance.
- How to speed-up the primal-dual iteration.

Thank you for the attention.

- Robert Beinert, Michael Quellmalz. Total Variation-based Reconstruction and Phase Retrieval for Diffraction Tomography. *SIAM Journal on Imaging Sciences*, to appear, 2022.